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Magnetic interlayer coupling and interaction between interface states in a quantum-well system

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Abstract. A first-principles Green's function technique has been used to investigate the magnetic interlayer coupling and the electronic structure responsible for the magnetic interaction in a bcc Fe/Cu_N/Fe system. We discuss the close relation between the interlayer coupling, the bulk Fermi surface of the spacer material, and the dispersion of the quantum-well states in the two-dimensional Brillouin zone. As a function of spacer thickness, we find an oscillatory long-range energy splitting of Fe/Cu interface states which is shown to be an example of a long-range oscillatory interface interaction transmitted by the spin-polarized quantum-well states of the Cu spacer. These interacting interface states may provide a signature of the magnetic coupling in multilayers.

1. Introduction

New techniques for obtaining tailor-made materials on an atomic scale have created fascinating possibilities for materials science. Superlattices and magnetic multilayers are two examples of artificial atomic-scale materials that can be produced with high precision and that have interesting properties such as an oscillatory magnetic interlayer coupling [1–3] and a giant magnetoresistance [4, 5]. One important feature of many of these layered metallic systems is the formation of two-dimensional quantum wells with confined electronic states, so-called quantum-well (QW) states [6–8], which are generally considered to be one of the major mechanisms behind the magnetic interlayer coupling [7, 9]. The occurrence of confined states within artificially prepared metallic devices with low symmetry has been observed in a variety of systems and may generally be understood in terms of quantum interference. In addition to the QW states, quantum-wire states have also been observed [11], and probably the most spectacular example is the direct observation of the confinement of surface states due to Fe adatoms forming geometrical patterns on a Cu(111) surface [12].

In the present paper we calculate the electronic structure and the magnetic interlayer coupling in Fe/Cu_N/Fe bcc (001) trilayers. In particular, we investigate the dispersion and the periodicity of the QW states confined within the spacer layers and their relation to the Fermi surface of the spacer bulk material. We also show how quasi-localized interface (IF) states at the Fe/Cu interfaces in the trilayer may interact via the spin-polarized QW states of the Cu spacer. This interaction is described in terms of hybridization and interference effects, and argued to be an example of a long-range interaction between IF states. We finally show how these interacting IF states may provide a signature of the magnetic interlayer coupling.

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Layered Fe/Cu bcc systems have been grown with the MBE technique [13–15] and are known to exhibit a characteristic oscillatory interlayer coupling [13–16, 18]. Fe/Cu bcc sandwiches is found to form an almost ideal QW system with confined QW states at the $\overline{\Gamma}$ point, periodically crossing the Fermi level as a function of the quantum-well width [19], similar to what is found for other magnetic multilayer systems [7, 8, 20]. Less attention has been devoted to the appearance of the QW states outside the $\overline{\Gamma}$ point, i.e. to the dispersion of the QW states in the two-dimensional Brillouin zone (2D BZ). Such a QW dispersion has in fact been measured for thin films of Cu on Co fcc (001) [21] and this provides a direct confirmation of the electronic structure governing the magnetic interlayer coupling.

The paper is organized as follows. In section 2 we briefly describe the calculational techniques used. In sections 3 and 4 we discuss the relation between the magnetic interlayer coupling and the dispersion of the QW states in the 2D BZ, and point out the relation to the Fermi surface of the spacer bulk material. In sections 5 and 6 we investigate the Fe/Cu IF states and their long-range interaction, which is described in terms of a coupling via the spin-polarized QW states. To study the interaction between IF states we compare the Fe/Cu_N/Fe bcc (001) trilayer consisting of two semi-infinite crystals of Fe separated by a paramagnetic Cu spacer with a Fe/Cu bcc (001) bilayer interface consisting of two semi-infinite crystals of Fe and Cu.

2. Method of calculation

The electronic structure calculations have been performed by means of the interface Green's function technique developed by Skriver and Rosengaard [22]. The method is based on the linear muffin-tin orbitals (LMTO) method [23, 24] within the tight-binding [25, 26], frozen-core, and atomic-sphere approximations together with the local spin-density approximation as parametrized by Vosko, Wilk, and Nusair [27]. It is a major advantage of the Green's function technique that it ensures a correct description of the loss of translational symmetry perpendicular to the interfaces without the use of an artificial slab or supercell geometry. Furthermore, the application of the principal-layer technique [28] to construct the interface Green's function leads to a numerically efficient technique in which the computer time scales linearly with the number of atomic layers. The method has been used in several studies of surface and interface properties [19, 29–33].

We calculate the magnetic interlayer coupling (IC), $E_{\mathrm{IC}}(N)$, as the difference between the total energy of the trilayer with the Fe magnetization aligned antiparallel on both sides, i.e., antiferromagnetic (AFM) alignment, and that of the trilayer with parallel magnetization, i.e., ferromagnetic (FM) alignment,

$$E_{\mathrm{IC}}(N) = E^{\mathrm{tot}}_{\mathrm{AFM}}(N) - E^{\mathrm{tot}}_{\mathrm{FM}}(N) \tag{1}$$

where N is the number of monolayers (ML) in the spacer. To investigate the properties of QW and IF states we study the spectral density function

$$D^{\sigma}(\boldsymbol{k}_{\parallel}, E) = \frac{1}{\pi} \operatorname{Im} \operatorname{Tr} G^{\sigma}(\boldsymbol{k}_{\parallel}, E) \tag{2}$$

calculated from the Green's function $G^{\sigma}(\boldsymbol{k}_{\parallel}, E)$ of spin σ, wave vector $\boldsymbol{k}_{\parallel}$, and energy E. Layer- and symmetry-resolved spectral density may be obtained by restricting the trace to single atomic layers or orbitals of specific symmetries. The Green's function on the real-energy axis may be calculated by means of analytical continuation from a linear mesh below the real axis in the complex-energy plane. When integrated over the 2D BZ, the k-resolved spectral density yields the total density of states (DOS).

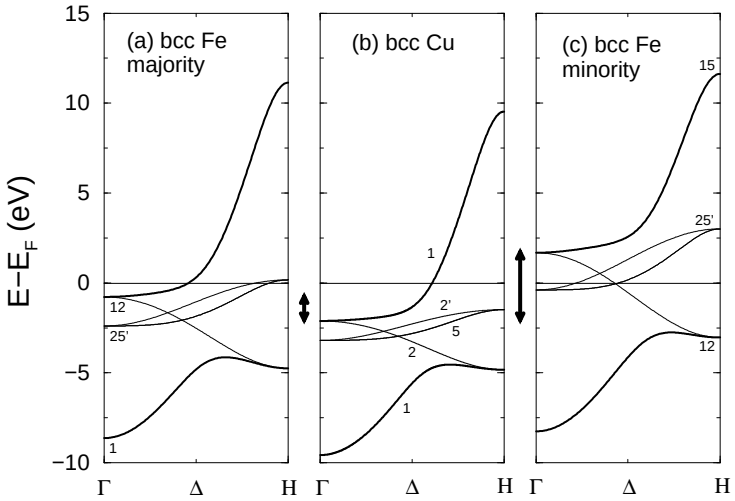

Figure 1. The bulk bands of bcc Fe and Cu along Γ–H. The arrows indicate the energy range in which magnetic quantum wells may be formed.

3. Quantum-well effects

3.1. The formation of QW states

The formation of magnetic quantum-well states in an Fe/Cu/Fe trilayer may be explained in terms of the bulk bands of bcc Fe and Cu, shown in figure 1, which correspond to the centre $\overline{\Gamma}$ of the 2D BZ. Of particular interest are states in the Cu band, Γ_{12}–Δ_1–H_{15}, which cannot scatter into the Fe majority band in the energy range from Γ_{12}(Cu) to Γ_{12}(Fe↑) and into the Fe minority band in the energy range from Γ_{12}(Cu) to Γ_{12}(Fe↓) because there are no available states of Δ_1 symmetry. As a result, majority-spin electrons with energies from -2.1 eV to -0.8 eV and minority-spin electrons with energies from -2.1 eV to 1.7 eV experience total reflection at the Fe–Cu interfaces and will therefore be confined to the Cu spacer and form QW states.

In the phase accumulation picture [34] one describes the confinement of QW states of wave vector $k_n^\perp$ as a condition for constructive interference, i.e.,

$$2k_n^\perp D + \varphi_L + \varphi_R = 2\pi n \tag{3}$$

where D is the spacer thickness, $\varphi_{L\,(R)}$ the reflection phase shift at the left, L, and right, R, interface, and n an integer quantum number. For a bcc (001) trilayer this leads to

$$k_n^\perp = (2\pi n - \varphi)/Na \tag{4}$$

where N is the number of atomic layers in the spacer, a the bcc lattice constant of the spacer material, and $\varphi \equiv \varphi_L + \varphi_R$. This relation specifies the quantization of the bulk bands of the spacer material embedded in a quantum well in terms of $k_n^\perp$. QW states of this kind have in fact been observed in several experiments [6–8, 35].

3.2. The QW dispersion and the Fermi surface

Due to the formation of QW states there will be sharp resonances in the spectral density of a trilayer. These resonances will occur not only at the $\overline{\Gamma}$ point but also throughout the 2D BZ.

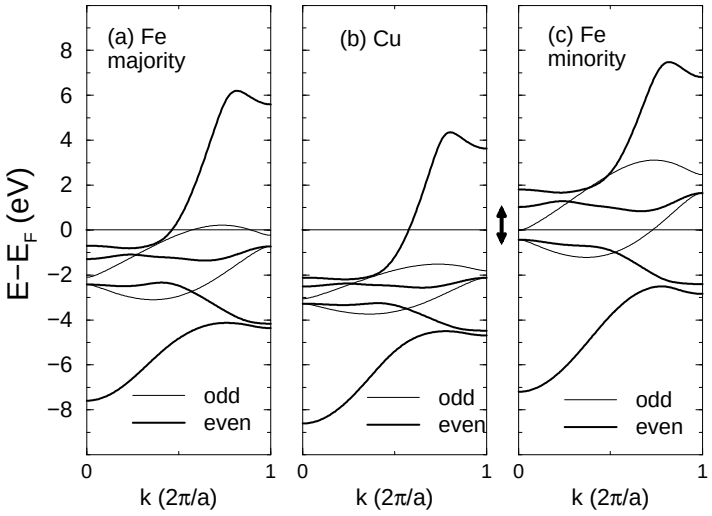

Figure 2. The bulk bands of bcc Fe and Cu along $\frac{\pi}{2a}(1, 0, 0)$–$\frac{\pi}{2a}(1, 0, 1)$. The arrow indicates the energy range in which a magnetic quantum well may be formed.

In figure 2 we show the bulk bands of bcc Fe and Cu for a low-symmetry line, $\frac{\pi}{2a}(1, 0, 0)$ to $\frac{\pi}{2a}(1, 0, 1)$, which corresponds to a point on a symmetry line in the 2D BZ. Here the symmetries are even or odd with respect to reflections in the [010] plane, and again we find a partial band gap for the minority-spin channel near the Fermi level. Quantum-well states will thus not only form at the $\overline{\Gamma}$ point but also in a large part of the 2D BZ, and the quantization condition (4) may be applied throughout the entire zone.

To obtain a simple understanding of the dispersion of the QW states in the 2D BZ we apply the bulk band-quantization condition in combination with a linearization of the bulk bands. That is, we assume that the quantized bulk band states

$$\varepsilon_{\mathrm{qw}}^{k_n^\perp}(\boldsymbol{k}_\parallel) = \varepsilon(k_n^\perp, \boldsymbol{k}_\parallel)$$

may be linearized around the Fermi wave vector $k_{\mathrm{F}}^\perp(\boldsymbol{k}_\parallel)$ and find that

$$\varepsilon_{\mathrm{qw}}^{k_n^\perp}(\boldsymbol{k}_\parallel) - \varepsilon_{\mathrm{F}} \approx (k_n^\perp - k_{\mathrm{F}}^\perp(\boldsymbol{k}_\parallel)) \frac{\partial \varepsilon}{\partial k^\perp}\bigg|_{k^\perp = k_{\mathrm{F}}^\perp} \tag{5}$$

which may be used to analyse the QW dispersion and especially the connection between the dispersion of the QW states and the Fermi surface of the bulk spacer material. From the linearization we find that the energy dispersion of a certain QW state, $\varepsilon_{\mathrm{qw}}^{k_n^\perp}(\boldsymbol{k}_\parallel)$, close to the Fermi level should resemble the shape of the Fermi surface $k_{\mathrm{F}}^\perp(\boldsymbol{k}_\parallel)$ provided that the band velocity $(\partial\varepsilon/\partial k^\perp)|_{k^\perp = k_{\mathrm{F}}^\perp}$ and the reflection phase shift φ in equation (4), which may depend on $\boldsymbol{k}_\parallel$, do not vary too rapidly.

To investigate the relation between the QW dispersion and the Fermi surface, we compare the cut of the bcc Cu Fermi surface in the $k_y = 0$ plane, shown in figure 3, with the calculated dispersion of the minority-spin spectral density of the Cu spacer along the $\overline{\Gamma}$–$\overline{\mathrm{X}}$ direction in the 2D BZ for a Fe/Cu_{15}/Fe trilayer, shown in figure 4. It is seen that QW states exist in a large part of the 2D BZ and that the spectral density shows several branches of QW resonances close to the Fermi level. It is also seen that the dispersion of the QW branches close to the Fermi level is very similar to the shape of the Fermi surface shown in figure 3 in agreement with equation (5). In particular, we note that the extremal points of the Fermi surface and

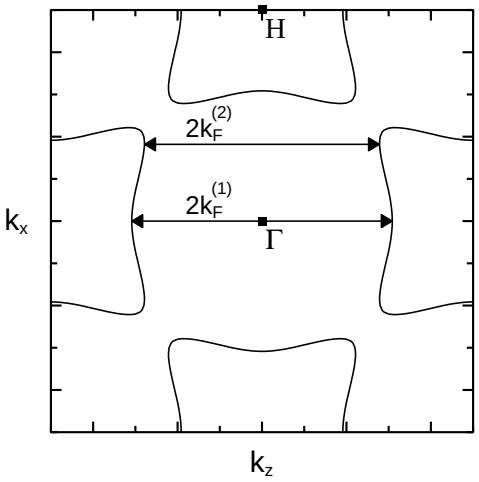

Figure 3. A cross section of the Fermi surface of bcc Cu in the $k_y = 0$ plane. The arrows indicate the stationary points of the Fermi surface.

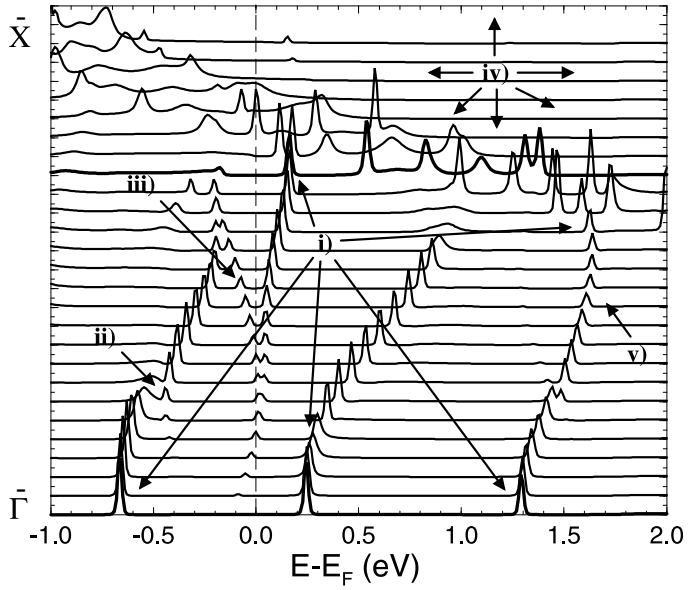

Figure 4. The minority-spin spectral density along $\bar{\Gamma}$–$\bar{X}$ in the 2D BZ summed over all Cu spacer layers of a Fe/Cu_{15}/Fe bcc (001) trilayer. The thick lines correspond to the $\boldsymbol{k}_\parallel$ for the stationary points of the Fermi surface.

the extremal points of the QW branches close to the Fermi level occur at the same $\boldsymbol{k}_\parallel$, i.e., at $k_x = 0$ ($k_y = 0$) in the 3D BZ corresponding to $\overline{\Gamma}$ in the 2D BZ and at the 'neck' extrema where $k_x = 0.7\pi/a$ ($k_y = 0$) both in the 3D BZ and in the 2D BZ. The extremal points are indicated by arrows, $2k_F^{(1)}$ and $2k_F^{(2)}$, in figure 3 and by two thick lines in figure 4. This relation between the Fermi surface and the quantum-well dispersion turns out to be very fruitful for the understanding of the connection between the periods of magnetic interlayer coupling and the Fermi surface of the spacer material.

There are a number of interesting features in the QW dispersions shown in figure 4, labelled (i)–(v), which deserve some comments. There are several extremal points labelled (i) in the QW dispersion which correspond to stationary points of the bulk Fermi surface as discussed above. These extrema will lead to van Hove singularities in the DOS and are therefore of particular importance for the electronic structure of the spacer material. In the region of energy and $\boldsymbol{k}_{\parallel}$ labelled (ii) the overlap between the Cu and Fe states is increased, due to the high spectral density in Fe, and the QW states disappear. In the region (iii) we observe a branch which does not follow the trend established by the branches. This branch corresponds to IF states and will be discussed below in section 5. The region labelled (iv) is devoid of Cu states and hence no QW states exist. Finally, we observe sharp resonances labelled (v) indicating that QW states are still formed above the actual partial gap shown in figure 2. These resonances exist due to the relatively small overlap between the states in Cu, with mainly sp character, and the d-like states in the narrow, second-highest even band in the Fe minority-spin channel.

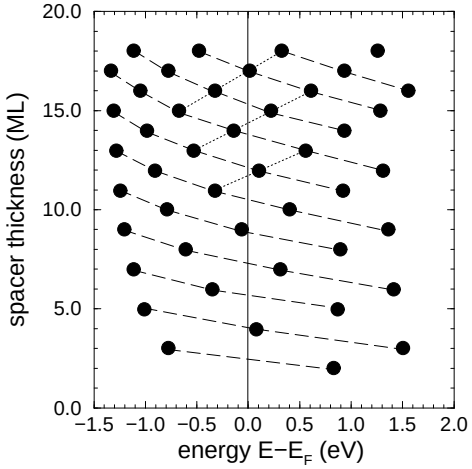

Figure 5. The minority-spin energy levels of the magnetic QW in Fe/Cu$_N$/Fe at the $\bar{\Gamma}$ point as a function of spacer thickness. The dashed lines indicate the 'dispersion' for a continuous change in the spacer thickness and the dotted lines indicate the 'dispersion' due to the aliasing effect.

3.3. The periodicity of QW states

The energy of a particular QW state decreases with increasing width of the quantum well and the QW states will therefore cross the Fermi level periodically, as the spacer thickness is changed. The period, P, of the Fermi-level crossing for a 'continuous' change of the width of the quantum well may be obtained from equation (4) as the spacer thickness difference, $N_2 - N_1$, in units of monolayers (ML) between two adjacent QW states, n_1 and n_2, at the Fermi level, i.e.

$$P = N_2 - N_1 = \frac{2\pi}{a}\frac{(n_2 - n_1)}{k_{\mathrm{F}}^{\perp}} = \frac{2\pi}{a}\frac{1}{k_{\mathrm{F}}^{\perp}}. \tag{6}$$

In figure 5 we show the energy distribution of QW states obtained from the spectral density at the $\overline{\Gamma}$ point as a function of spacer thickness where the dashed lines indicate the periodicity from a hypothetical continuous change of the spacer width. The calculated QW states are passing the Fermi level with a periodicity of around 1.6–1.7 ML for thick spacers. This is

in good agreement with the periodicity of 1.62 ML obtained from the periodicity relation equation (6) together with the calculated Cu bulk Fermi wave vector.

Due to the discreteness of the spacer lattice the QW energies in figure 5 are sampled only at integer numbers of spacer layers. When $k_{\mathrm{F}}^{\perp} > \pi/a$ one therefore may see another type of periodicity, which is usually referred to as the aliasing effect. In this case the period is

$$P = 1\Big/\left(1 - \frac{a}{2\pi}k_{\mathrm{F}}^{\perp}\right) \tag{7}$$

and the energy of the QW states will appear to increase with increasing spacer width. The dotted lines in figure 5 indicate the periodic appearance of the QW states due to the aliasing effect. The periodicity of the QW states in this case is approximately 2.6 ML for thick spacers, which is in perfect agreement with the periodicity of 2.61 ML extracted from equation (7). This shows that the periodic behaviour of the QW states is essentially governed by the bulk properties of the spacer bulk material.

4. The magnetic interlayer coupling

Of particular interest for the periodic behaviour of the electronic structure are the extremal points of the QW dispersion marked (i) in figure 4. The van Hove peaks in the total DOS centred near these extrema will cross the Fermi level with the periodicity given by equation (7) where the Fermi wave vector is extracted from the corresponding extrema of the bulk Fermi surface. The band energy with respect to the Fermi level

$$E_{\mathrm{band}} = \sum_{\sigma}\int^{\varepsilon_{\mathrm{F}}} (\varepsilon - \varepsilon_{\mathrm{F}})D^{\sigma}(\varepsilon)\,\mathrm{d}\varepsilon \tag{8}$$

and thus a major part of the magnetic interlayer coupling

$$E_{\mathrm{IC}} \approx E_{\mathrm{band}}^{\mathrm{AFM}} - E_{\mathrm{band}}^{\mathrm{FM}} = \sum_{\sigma}\int^{\varepsilon_{\mathrm{F}}} (N_{\mathrm{FM}}^{\sigma}(\varepsilon) - N_{\mathrm{AFM}}^{\sigma}(\varepsilon))\,\mathrm{d}\varepsilon \tag{9}$$

(where $D^{\sigma}(\varepsilon)$ is the DOS and $N_{\mathrm{AFM}}^{\sigma}(\varepsilon)$ the number of states) will therefore consist of a superposition of oscillations with the periods corresponding to the extremal points of the bulk Fermi surface.

The amplitude of the oscillations in the DOS as well as in the magnetic interlayer coupling will depend on the curvature of the QW dispersion. The curvature essentially corresponds to the band mass at the stationary points of the Fermi surface of the bulk spacer material as assumed in the stationary-phase approximation of the RKKY theory [40] as well as in the QW theory [9]. However, it is the stationary points of the QW dispersion which are important for the electronic structure and interlayer coupling, and not the somewhat artificially introduced bulk Fermi surface, which does not exist for a finite spacer. On the other hand, the bulk Fermi surface has a structure and shape similar to the QW dispersion, and is therefore related to the periodic behaviour of the QW states and the oscillations in the band energy and the magnetic interlayer coupling in the thick-spacer limit. However, the QW dispersion in the 2D BZ is the more direct quantity to consider in the investigation of the interlayer coupling, in particular in view of the fact that it may be measured by means of angle-resolved photoemission [21].

In figure 6 we present the magnetic interlayer coupling $E_{\mathrm{IC}}(N)$ calculated for Fe/Cu_N/Fe trilayers by means of equation (1) together with a least-squares fit to an RKKY-like expression for the magnetic interlayer coupling in the limit of thick spacers:

$$E_{\mathrm{RKKY}}(N) = \frac{1}{(Nd)^2}\sum_{i=1}^{2} A_i \cos\left(\frac{N}{P_i}2\pi + \delta_i\right). \tag{10}$$

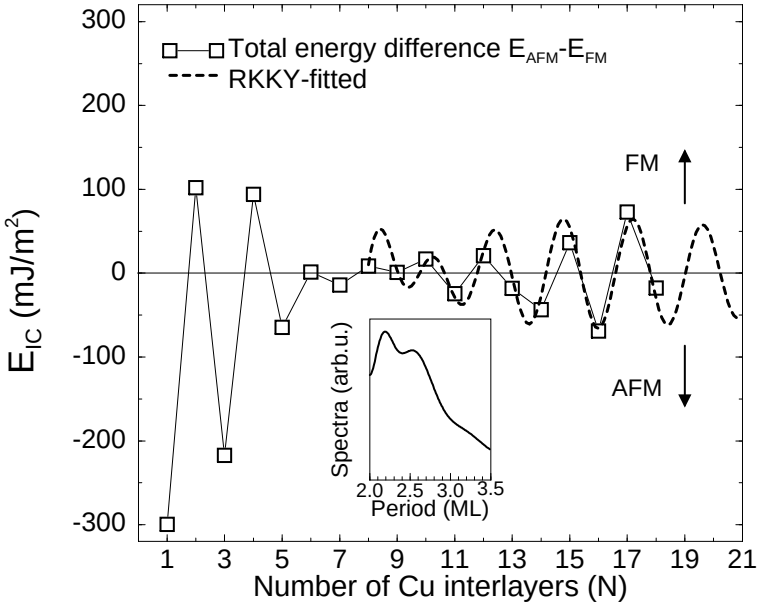

Figure 6. The magnetic interlayer coupling as a function of spacer thickness for a Fe/Cu/Fe bcc (001) trilayer. The dashed curve shows the coupling energies obtained in a least-squares fit to the RKKY expression in equation (10) with two superposed oscillations in the range from 8 to 18 ML. The inset shows the Fourier spectrum, $|A(P)|^2$ in equation (11), of the interlayer coupling from 1 to 18 ML.

Table 1. The periods P_1 and P_2 in units of monolayers (ML) extracted from the magnetic interlayer coupling (IC), the extremal points of the Fermi surface (FS) and the quantum-well states crossing the Fermi level (QW).

	IC	FS	QW
P_1 ($\overline{\Gamma}$)	2.6 ML	2.61 ML	2.6 ML
P_2 (neck extrema)	2.3 ML	2.26 ML	2.2 ML

Here, N is the number of monolayers (ML), P_i the periodicity in units of monolayers, d the thickness of a monolayer and δ_i a phase shift.

According to RKKY theory the periods, P_i, in the asymptotic limit are given by vectors separating the stationary points of the Fermi surface of the spacer material. Two spanning vectors are shown in figure 3 as $2k_F^{(1)}$ and $2k_F^{(2)}$, and the relation between the periods P_i and the Fermi wave vectors $k_F^{(2)}$ is given by (7) where the aliasing effect is taken into account. Contributions from stationary points of bcc Cu corresponding to the $\overline{\mathrm{M}}$ point in the 2D BZ [10] were not found in the interlayer coupling. This can be understood from the fact that there is no gap in Fe around this point. In table 1 the periods extracted by the least-squares fitting of the magnetic interlayer coupling in figure 6 are compared with the periods calculated both from the stationary points of the Fermi surface and the periods with which the QW states cross the Fermi level. It is seen that the periods extracted from the calculated interlayer coupling are very much consistent with the periods extracted from the Fermi surface, in accordance with RKKY as well as QW theory. The periodicity of the interlayer coupling is also in very good agreement with the periodicity of the QW states at the stationary points of the QW dispersion. However, the agreement may be somewhat fortuitous since the RKKY periods were obtained

in a fit to the calculated magnetic interlayer coupling in the long-range limit from 8 to 18 ML. This choice is rather arbitrary and the periods extracted are sensitive to small variations in the range, probably due to pre-asymptotic behaviour. The different periods may alternatively also be compared with the periods of a discrete Fourier transform in the full range from 1 to 18 ML of the interlayer coupling:

$$A(P) = \frac{1}{N_{\max}} \sum_{N=1}^{N_{\max}} N^2 J(N) \exp^{-\mathrm{i}\, 2\pi N/P} . \tag{11}$$

The Fourier spectrum, $|A(P)|^2$, as a function of the period P in units of ML, shown in the inset of figure 6, has only two peaks for the periods 2.2 ML and 2.5 ML. These periods are only slightly shorter than those extracted from the least-squares fit.

The periods of the calculated interlayer coupling in figure 6 may be compared with experiments [13, 15] as well as with earlier calculations [16]. Heinrich *et al* [13] measured the interlayer coupling in the range between 6 and 12 ML of Cu in a Fe/Cu/Fe bcc (001) trilayer sandwich and found only a single change from FM to AFM coupling between 9 and 10 ML of Cu. The failure to observe short-range oscillations may be due to interface roughness which tends to suppress such periods [36–39]. The experiment performed by Johnson *et al* [15] for the range of 10 to 19 ML of Cu shows AFM coupling near 12, 14, 16 and 18 ML of Cu. This is in excellent agreement with the present calculations, which indicates that not only the periods but also the phases are in agreement. However, one should note that a quantitative comparison with experiment can be very uncertain, not least due to the imperfections in the artificially prepared Cu bcc spacer which may destroy the coherence of the QW states mediating the coupling. In an earlier calculation by Krompiewski *et al* [16] almost perfect agreement with the experiments by Heinrich *et al* [13] was found. However, the calculations were performed for a periodic multilayer system and the calculated interface coupling was strongly influenced by the thickness of the Fe layers. In fact, the interface coupling did not seem to be fully converged even for an Fe thickness of 16 ML and the comparison with the trilayer system is therefore uncertain. A more recent trilayer calculation by Costa *et al* [17], where temperature effects are taken into account, showed an oscillatory behaviour of the interlayer coupling with a period of about 2.5 ML.

In the literature there is a wide spread in the reported coupling strengths. Our calculated coupling amplitude is larger than those found in experiments. The feature that calculations always seem to give a stronger coupling is usually explained as due to imperfections in the samples used in experiments which weaken the observed coupling.

5. Interface states

In connection with the discussion of the dispersion of the QW states in figure 4 we encounter a branch which does not follow the trend expected for a QW state. The origin of this branch becomes clear when we consider the minority-spin spectral density for an Fe/Cu bilayer projected onto the atomic layers adjacent to the interface shown in figure 7. Here, we observe a branch of the spectral density which decays rapidly as one moves away from the interface and, hence, corresponds to interface states. Such IF states, locally confined to a few atomic layers near the interface, may generally arise when there are symmetry-dependent partial band gaps in the bulk of the two metals forming the interface.

In the present case, the IF states are directly related to well-known minority-spin surface states of bcc Fe [41–43]. While a partial band gap exists in the minority-spin bands of bcc Fe, as is seen in figure 2, there is no band gap of the relevant symmetry in bcc Cu. However, the Fe IF states, which are mainly of d character, hybridize only weakly with sp bands of Cu, and

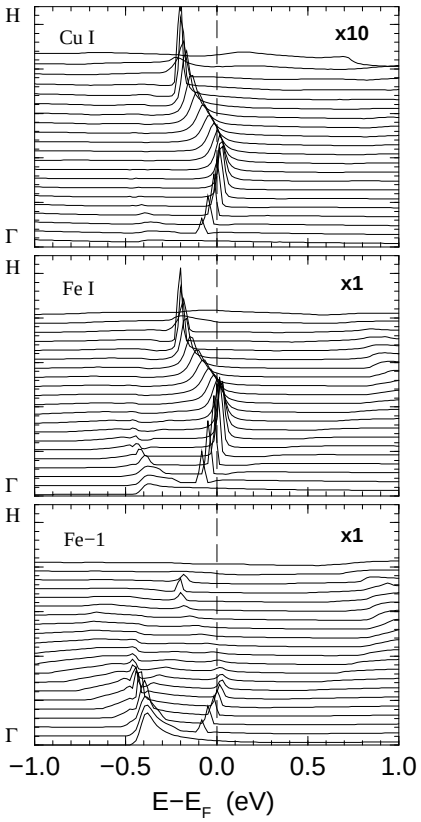

Figure 7. The layer-resolved minority-spin spectral density for a Fe/Cu bcc (001) bilayer consisting of two semi-infinite crystals of bcc Fe and bcc Cu. The IF states close to the Fermi level in the Fe interface layer, Fe I, decay rapidly as they move away from the interface. Notice the change in scale in the upper panel (×10).

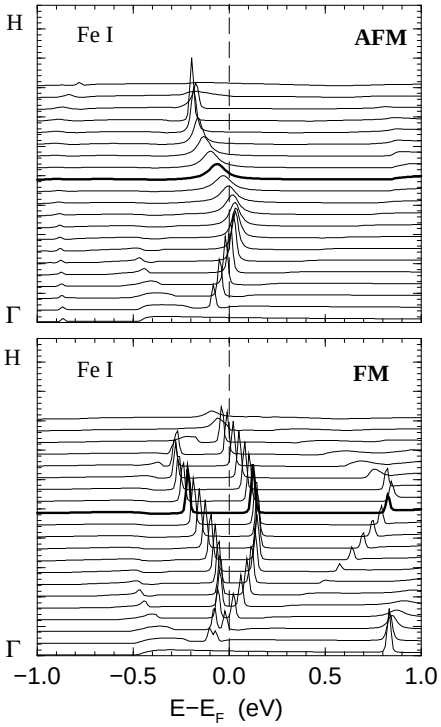

Figure 8. The layer-resolved minority-spin spectral density for a $Fe/Cu_2/Fe$ bcc (001) trilayer with the Fe magnetization aligned parallel (FM) and antiparallel (AFM). In the FM case the IF states split into two bands of bonding and antibonding states. The bold curves show the spectral density for $\boldsymbol{k}_{\parallel} = (\pi/2a, 0)$.

hence form virtual bound states that are fairly well localized at the interface. If the IF state occurs at one of the extrema of the QW dispersion, an interaction between the IF and QW states will strongly influence the interlayer coupling. In the following we therefore study the IF state in more detail.

6. Interaction between interface states

When two bilayers are brought together to form a trilayer, the IF states of the two interfaces may interact. One example of such an interaction may be found in figure 8 where we show the local minority-spin spectral density in a $Fe/Cu_2/Fe$ bcc (001) trilayer at the Fe interface layer (Fe I), for AFM as well as FM coupling. It is seen that only in the FM case do the IF states split into two bands. The reason for this is that in the AFM case the two spin-polarized IF states located at each of the two interfaces belong to different spin channels and hence do not interact. The splitting of the IF state in the FM case may be regarded as the formation of bonding and antibonding states due to an overlap with the spin-polarized IF state situated at

the other interface. Since the splitting does not occur for an AFM alignment, the existence of a splitting will be a signature of a FM interlayer coupling. Measurements of the IF states may therefore provide a direct way of determining the spin alignment in magnetic multilayers.

Since an interaction between localized IF states is expected to decay as a function of increasing spacer thickness due to the decreasing overlap, one might assume that the splitting would disappear for spacers of more than a few atomic monolayers. However, in the present case where the IF states are only quasi-localized on the Cu side of the interface, the interaction is strongly influenced by the QW states. In fact, the existence of a partial gap in Fe (see figure 2), which, on the one hand, gives rise to the quasi-localized IF states, due to the weak hybridization with the sp-like states in Cu, and, on the other hand, gives rise to the QW states in the spacer, is crucial for such an interaction between IF and QW states.

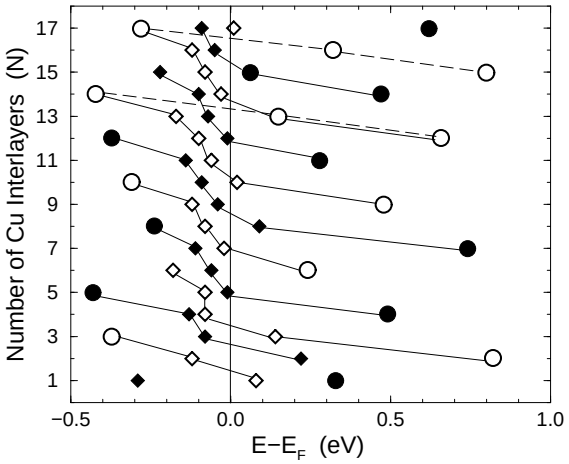

Figure 9. The minority-spin QW states and Fe/Cu IF states for the Fe/Cu$_N$/Fe bcc (001) trilayers as a function of the spacer layer thickness N for $\boldsymbol{k}_\parallel = (\pi/2a, 0)$. Diamonds show the positions of the states which are mainly localized to the Fe/Cu interface, i.e., IF states, and the circles show the energies of the states extended over the full spacer layer, i.e., QW states. The dashed lines are guides to the eyes to show the 'dispersion' of QW states. The full lines connect states of the same kind of symmetry, empty symbols for odd states and filled ones for even states.

In figure 9 we show the positions of the peaks in the minority-spin spectral density for $\boldsymbol{k}_\parallel = (\pi/2a, 0)$ as functions of the spacer layer thickness. Each state has been identified as either a QW state (circle) or an IF state (diamond) by means of the character of the layer-projected spectral density. The QW states are taken to have a significant weight in the central part of the Cu layer while the IF states are assumed to be localized to the interfaces. In some cases, e.g., for 3 and 15 atomic layers, the assignment is somewhat ambiguous since the QW and IF states are strongly mixed. The 'dispersion' of pure QW branches, which is indicated by dashed lines for a few cases, is seen to be perturbed by crossing IF states. The corresponding perturbation of the QW dispersion in reciprocal space is clearly seen at (iii) in figure 4. The mixing repels all QW states in an energy range close to the IF states, and simultaneously leads to an oscillatory splitting of the IF states which follows the periodic dispersion of the QW states. Since there exist bands of QW and IF states in the 2D BZ (see figures 4, 7 and 8), this splitting occurs not only at $\boldsymbol{k}_\parallel = (\pi/2a, 0)$, which is chosen here as an illustrative example, but also in an extended area of the 2D BZ.

In figure 10 we display the splitting energy for the IF state at $\boldsymbol{k}_\parallel = (\pi/2a, 0)$ as a function of the spacer thickness. For thin spacers, up to four monolayers, the coupling decays rapidly, as

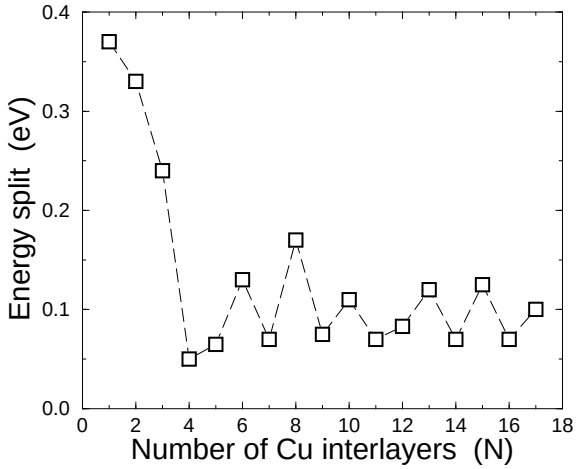

Figure 10. The splitting energy for Fe I IF states at $\boldsymbol{k}_{\parallel} = (\pi/2a, 0)$ in Fe/Cu_N/Fe bcc (001) trilayers as a function of atomic spacer thickness N.

expected for a decreasing overlap between the IF states. For larger spacer thicknesses however, the energy splitting oscillates around a value of approximately 0.1 eV. This oscillatory long-range splitting of the IF states is directly related to the interaction with the QW states that periodically cross the IF state as was shown in figure 9.

A detailed analysis gives the following picture. Due to the inversion symmetry in the plane through the centre of the Cu spacer, all states are either even or odd with respect to reflection in this plane. In particular, the pair of split IF states consists of one even and one odd state. For a single monolayer spacer, where the splitting is related to the direct overlap, we find that the even state is bonding and the odd one is antibonding in accordance with a simple chemical bonding picture. In addition, the QW state has a specific reflection symmetry, every second state being either even or odd. Now a QW state and an IF state of the same symmetry will hybridize. This has several consequences:

(i) For spacer layers of more than a few monolayers, where the direct overlap between IF states is small, the QW states appear denser in energy. This leads to an increased hybridization between IF and QW states which prevents a rapid decay of the splitting energy.

(ii) If a QW state of a certain symmetry is close in energy to an IF state of the same symmetry, the hybridization between the QW IF states for the opposite symmetry is at the same time small. The energy of the IF states of this other symmetry is therefore essentially the same as for the IF state of the Fe/Cu bilayer which is -0.07 eV for $\boldsymbol{k}_{\parallel} = (\pi/2a, 0)$.

(iii) If a QW state of odd (even) symmetry is situated slightly above (below) the energy of the IF states, the 'bonding' IF state may actually be odd, in contrast to a simple diatomic molecule picture. Due to the periodic behaviour of the QW states, the symmetry of the two IF states will therefore, as a function of spacer thickness, vary in an oscillatory manner between odd and even.

An interesting phenomenon seen in figure 9 is the jumps which the branches connecting states of the same symmetry (full lines) exhibit when they cross the energy of the IF states. This is closely connected to the 'branch jumps' of the QW states in Co/Cu(001) trilayers with finite Co thickness [20], where confined d states of the Co layers play a role similar to that of the IF states in the present work. As discussed in reference [20], these branch jumps may be

understood in terms of the phase accumulation picture of equation (3). A QW state passing the energy region of the IF states, as the spacer thickness is increased or decreased, experiences a large shift in the reflection phases, φ_{L} and φ_{R}, due to the IF resonance. As a result, two extra nodes appear in the wave function of the QW state. This effect leads to branch jumps of the dispersion curve similar to those in figure 9. In the phase accumulation or interference picture, which is complementary to the hybridization interpretation above, we may thus regard the long-range interaction between the IF states as caused by the occurrence of QW IF resonance states, which are extended over the whole quantum well, however with the major weight still in the interface regions.

7. Summary and conclusions

The magnetic interlayer coupling and the electronic structure responsible for the magnetic interactions in the Fe/Cu bcc system has been studied by means of first-principles calculations. The dispersion of the QW states in the 2D BZ has been investigated as well as their periodic behaviour as a function of spacer thickness. The relation between the dispersion of the QW states, the bulk Fermi surface of the spacer material and the magnetic interlayer coupling has also been discussed. The periodicity of the interlayer coupling and the QW states were found to be in excellent agreement with the periods extracted from the stationary points of the bulk Fermi surface as expected from RKKY and QW theory. As a major result we find that the spectral density—especially the QW resonances and the corresponding QW dispersion—is a very powerful tool in the understanding of the electronic structure governing the magnetic interlayer coupling.

Furthermore, it has been shown how IF states in the spin-polarized quantum well may split as a function of magnetic alignment and spacer thickness. The splittings of the IF states only occur when the Fe magnetization is aligned in parallel, i.e., when the opposite IF states belong to the same spin channel. The IF state splitting is therefore directly related to the interlayer coupling which determines the magnetic alignment. As a function of spacer thickness the splitting energy decays rapidly for thin spacers and oscillates for larger spacer thicknesses. The short-range behaviour is directly related to the overlap between opposite IF states belonging to the same spin channel, whereas the oscillatory long-range behaviour is shown to be related to an indirect interaction transmitted via the QW states. What could be very interesting to investigate in future is to what extent the split interface states affect the magnetic anisotropy, which has a substantial contribution from the interfaces. These might give rise to a thickness-dependent oscillatory interface contribution to the anisotropy energy.

The QW states are responsible for the magnetic interlayer coupling as well as the splitting of the IF states. The characteristic appearance of the IF states is thus not only an interesting example of a long-range oscillatory interaction, but may also serve as a measure of the sign of the magnetic interlayer coupling. The indirect interaction between IF states, transmitted via QW states, as shown here for Fe/Cu bcc (001) multilayers, is expected to occur also in similar systems and the phenomenon is a direct consequence of the interaction of electronic states confined in different ways.

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